Direct Numerical Simulation of Turbulent Combustion

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At present, computational fluid dynamics (CFD) of turbulent combustion is considered as an important and reliable tool for developing modern combustion devices. Here, in addition to the standard complexities related to compressible nonreactive flows, other phenomena such as the heat release from the combustion reaction, the strong density fluctuation and the increase of the fluid viscosity, have to be taken into account. Conventional concepts used for the numerical computations of turbulent reactive flows are known as the Reynolds-averaged Navier-Stokes (RANS) approach or the large eddy simulation (LES) [1], which rely on modeling the underlying fundamental principles, i.e., turbulent flow, combustion reaction and their mutual interaction, with the help of statistical methods. The direct numerical simulation (DNS) on the other hand is much more expensive in computing time compared to the RANS or LES simulation, which relies on the exact formulation of the governing conservation equations, without implementing any additional empirical or statistical models. Hence, it can provide detailed insight into mechanisms occurring during the flame-turbulence interaction which strongly influence the efficiency of combustion processes. Accordingly, DNS of turbulent reactive flows are well suited for the development and validation of subordinate modeling concepts, for example, in the framework of RANS or LES.

To perform DNS of chemically reacting flows, conservation equations for the total mass, the momentum, the mass of each reacting species and the energy have to be solved altogether with the equation of state [1, 2]. In addition, depending on the complexity of the reaction mechanism and molecular diffusion model used, calculations of the reaction rates and diffusion fluxes may take a major part ($> 50\%$) of the total computing time due to the very expensive mathematical operations. This can easily overwhelm the available computational resources in both memory and time. In general, the choice of physical and chemical laws is determined by an efficient compromise between available computational resources and attainable accuracy. Additionally, the computational grid needed for DNS must be sufficiently fine in order to resolve the smallest existing length scales in the turbulent reactive flow, which are represented by the smallest turbulent vortices and the thickness of the flame front or the reaction zone, respectively [1]. Accordingly, a small time step has to be set to ensure numerical stability. As a consequence, an extremely high amount of computational time is required for the DNS of turbulent reactive flows. This is the main reason why DNS of combustion related problems is limited to fundamental research purposes until now. These are, for example, flows at a low Reynolds number (Re) or flows restricted to a simulation domain in the centimeter range or with only two-dimensions.

Recently, the tremendous progress in high performance computing (HPC) techniques on supercomputer facilities has enabled DNS of turbulent combustion for real-scale academical applications [3]. Nevertheless, most of the available DNS have been made on computational domains with simple geometrical shapes such as boxes or squares, for the simple reason that implementations of the related DNS solvers are highly specialized for such simple geometries or they cannot efficiently speed up with large numbers of processors. As an example by using the finite difference method (FDM) with an explicit time discretization or by restricting the mesh to be structured where the total number of CPU cores must correspond to the number of subdividing blocks and each block should ideally be allocated with the same number of computing cells. Furthermore, due to the fact that thousands of processors are used in parallel and that an optimal implementation for different high performance computing clusters is desired, commercial solvers or closed-source codes are not suited here. An objective of the current work is therefore to introduce a newly developed DNS solver that has been implemented into the open source program package OpenFOAM [4], which is suited for massive parallel computing of chemically reacting flows on computational grids with complex geometries.

In order to validate the applicability of the proposed solver, it has been used to simulate different types of flames, among them a laminar flat flame and a propagating turbulent flame front (Fig.1 and Fig.2). The first case is intended especially for the validation of the code with respect to the treatment of reaction kinetics and molecular transport fluxes, whereas the second case mainly aims to justify the capability of the code for three-dimensional problems. Subsequently, DNS of two real-scale combustion experiments, which are given by a propagating flame front in a bomb device (Fig.3) [5] and a turbulent jet flame (Fig.4)[6], have been performed, which employs two complex computational grid with 64 million and 111 million finite volumes. The DNS for these cases have been carried out in parallel with 4096 and 8192 processors on the Cray XE6 (HERMIT) and JUQUEEN (IBM Blue Gene/Q) clusters maintained by the High Performance Computing Center Stuttgart (HLRS) [7] and the Jülich Supercomputing Center (JSC) [8]. The results showed a very good agreement with the measured data. In addition, the solver has proved to speedup efficiently on these multiple massive high performance computers.

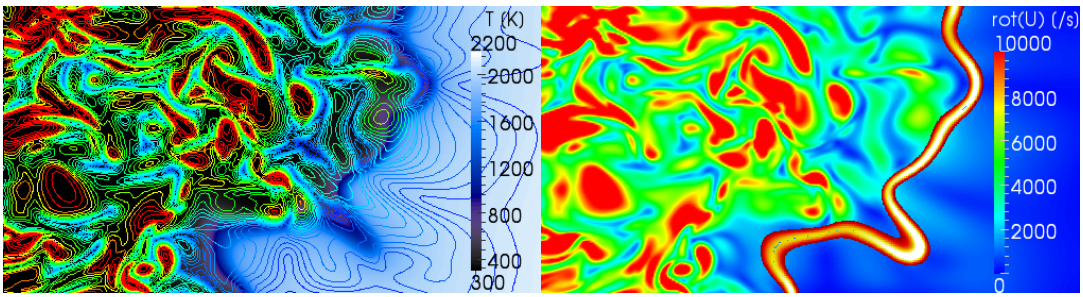

Figure 1: Interaction of the flame front with the turbulent flow: Iso-contours of the vorticity (left) and the heat release rate (right) with temperature and vorticity as backgrounds.

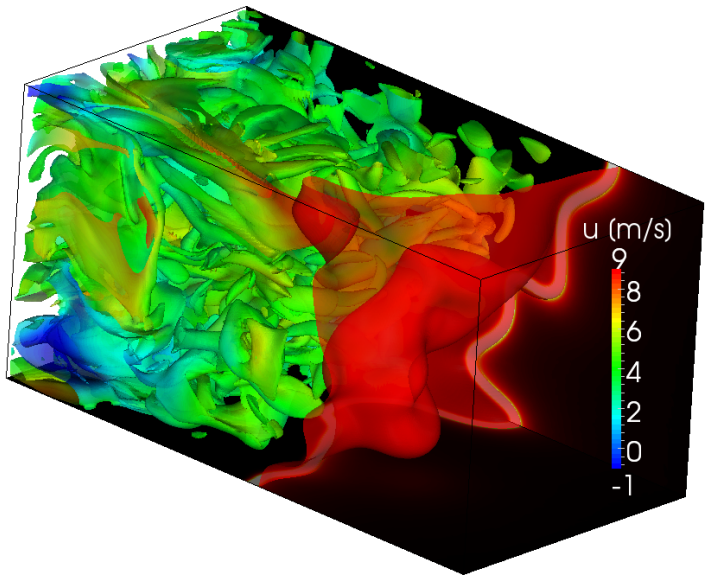

Figure 2: Three-dimensional DNS of a propagating flame front: iso-surfaces of the vorticity field and the temperature field.

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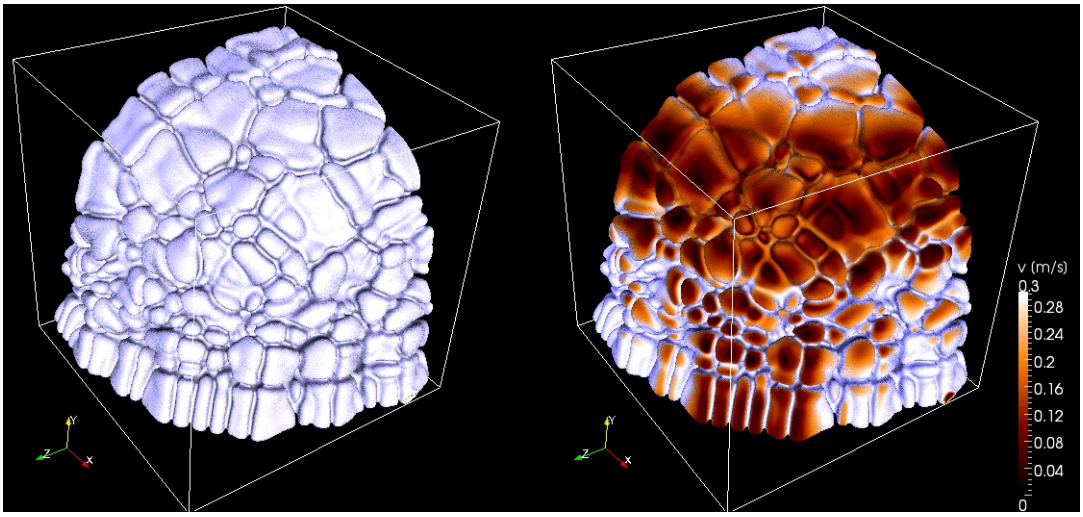

Figure 3: Three-dimensional DNS of collapse of a propagating flame front in a bomb vessel.

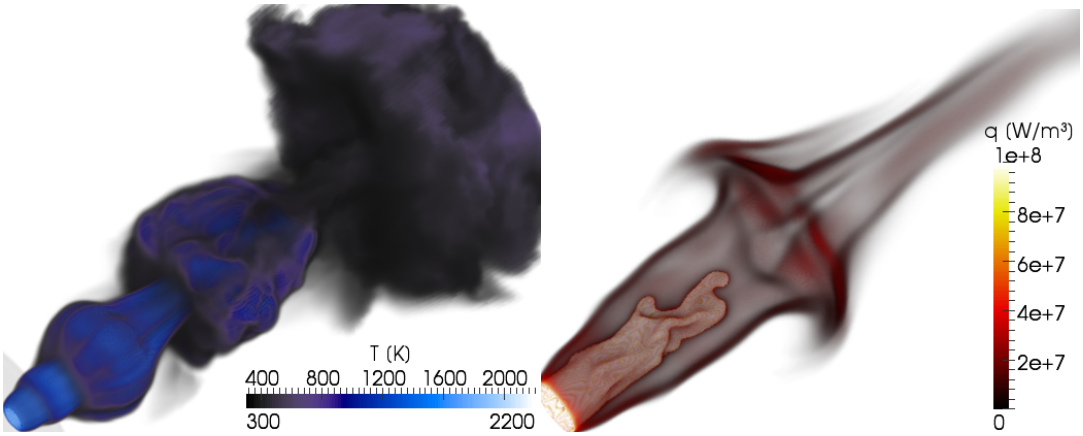

Figure 4: Three-dimensional DNS of a moderately turbulent jet flame: instantaneous volume rendering of temperature (left) and heat release rate (right).

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